

Predicting the hybridization state: a comparative study between conventional and innovative formulae

Arijit Das

Department of Chemistry, Bir Bikram Memorial College, India

Article Info

Article history:

Received Sep 11, 2019
Revised Nov 7, 2019
Accepted Jan 1, 2020

Keywords:

Chemical education research
Hybridization
Graduate student
Post graduate student
Under graduate student

ABSTRACT

In previous published articles, formulae-based mnemonics by counting the total number of σ bonds with a lone pair of electrons (LP), a localized negative charge (LNC), or a localized lone pair of electrons (LLP) and subtracting one (01) from this total value (T_{SLP} , T_{SLNC} , or T_{SLLP}) to predict the power of the hybridization state of simple molecules or ions and organic compounds, including heterocyclic compounds have been discussed. These are the innovative and time-efficient methods of enhancing student interest. Here, in this new article, the limitations of conventional formulae in comparison to the use of innovative formulae have been discussed along with the application of the hybridization state in different fields of chemical education. This article encourages students to solve multiple choice type questions (MCQs) at different competitive examinations in a time economic ground on the prediction of hybridization state of simple molecules or ions to know their normal and subnormal geometry and prediction of hybridization state of hetero atom in different heterocyclic compounds to know the planarity of the compounds, which is very essential factor for prediction of aromaticity of heterocyclic compounds. Educators can use this comparative study in their classroom lectures to make chemistry authentic and intriguing. Because the use of mnemonics in classroom lectures is an essential tool to become a distinguished educator.

This is an open access article under the [CC BY-SA](#) license.



Corresponding Author:

Arijit Das,
Department of Chemistry,
Bir Bikram Memorial College,
College Street Road, Agartala, Tripura, India 799004.
Email: arijitdas78chem@gmail.com

1. INTRODUCTION

Conventional formulae by using conventional methods [1-20] for the prediction of hybridization state of simple molecules or ions, organic compounds including different heterocyclic compounds containing one, two or more number of hetero atoms is mystifying and time consuming. Keeping this in mind, I have introduced formulae-based mnemonics by counting the total number of σ bonds with a lone pair of electrons (LP), a localized negative charge (LNC), or a localized lone pair of electrons (LLP) and subtracting one (01) from this total value (T_{SLP} , T_{SLNC} , or T_{SLLP}) to predict the power of the hybridization state of simple molecules or ions and organic compounds, including heterocyclic compounds [21-27].

Conventional formula for the prediction of hybridization state of simple molecules or ions and hetero atom in different heterocyclic compounds had wide limitations in the field of both organic and inorganic chemistry which were misguided by the educators since last 80-90 years. In this article, I have tried to focus the limitations of conventional formula to predict the hybridization state of center atom in simple molecules or ions and also in the organic compounds in and solved them in the light of innovative formulae.

2. FORMULAE BASED METHODOLOGIES

2.1. Conventional formulae

Conventional formulae using conventional methods [1-20] for the prediction of the hybridization state:

The hybridization state for a molecule can be calculated using $P = 1/2 (V + MA - C + A)$, where V = the number of valance electrons in the central atom, MA = the number of surrounding monovalent atoms, C = cationic charge, A = anionic charge, and P = power of the hybridization state.

2.2. Innovative formulae-1

An innovative formula [21-23, 25-27] for predicting the hybridization state of simple molecules or ions:

The power of the hybridization state of the central atom is $(P_{Hyb}) = (T_{SLP}) - 1$,

Where P_{Hyb} = power of the hybridization state of the central atom, T_{SLP} = (total number of σ bonds around each central atom + LP).

In order to work out a molecule's Lewis structure, first predict the number of sigma bonds (σ -bonds), pi bonds (π -bonds), and the lone pair of electrons (LP), if any. All single (-) bonds are σ bonds, while 1σ and 1π are the double bond (=), and 1σ and 2π (exclude π bond) form the triple bond (\equiv). In addition to these, each co-ordinate bond (\rightarrow) can be treated as a 1σ bond. This formula is applicable up to four (04) T_{SLP} .

If the power of the hybridization state (P_{Hyb}) is 03, 02, and 01 then the hybridization state will be sp^3 , sp^2 , and sp , respectively.

2.3. Innovative formulae-2

An innovative formula [21-27] for predicting the hybridization state of carbon atom in different organic compounds:

Power of the hybridization state in the central atom, $(P_{Hyb}) = (T_{SLNC}) - 1$

Where P_{Hyb} = power of the hybridization state of the central atom, and T_{SLNC} = (total number of σ bonds around each central atom + localized negative charge).

All single (-) bonds are σ bonds, while 1σ and 1π are the double bond (=). Also, (LNC) = localized negative charge. A negative charge bearing carbon atom in the ring system of the organic compound when directly attached with single and double bonds is considered to be an LNC containing carbon atom and its negative charge is to be treated accordingly.

2.4. Innovative formulae-3

An innovative formula [22-24] for predicting the hybridization state of the heteroatom in different heterocyclic compounds:

Power of the hybridization state of a heteroatom $(P_{Hyb}) = (T_{SLLP}) - 1$,

Where P_{Hyb} = power of the hybridization state of the heteroatom, T_{SLLP} = (total number of σ bonds around each central atom + LLP), and LLP = localized lone pair of electrons. If the power of the hybridization state (P_{Hyb}) is 03, 02, and 01 then the hybridization state will be sp^3 , sp^2 , and sp , respectively. All single (-) bonds are σ bonds, while in a double bond (=) there is one σ and one π . The heteroatom (an atom containing a lone pair of electrons), which is directly attached with single and double bonds using the ring system, is considered to be an LLP-based heteroatom and its lone pair is to be treated as a localized lone pair of electrons (LLP).

3. RESULTS AND ANALYSIS

3.1. Comparative study between conventional and innovative formulae for the prediction of the hybridization state of different atoms in simple molecules or ions.

When using a conventional formula, it is not possible to predict the hybridization state of an O atom in the cyclic ozone, as illustrated in Figure 1

Example 1: The hybridization state of O in cyclic ozone

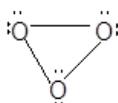


Figure 1. Equilateral triangle structure of cyclic ozone (O_3)

Conventional formula: $P = 1/2 (V+MA-C+A) = 1/2 (6+0-0) = 3.0$ (sp^2 - erroneous hybridization state of O)

Innovative formula: $(P_{Hyb}) = (T_{SLP}) - 1 = (2+2)-1 = 3$ (sp^3 hybridized O atom in cyclic ozone)

Where P_{Hyb} = power of the hybridization state of the central atom, and T_{SLP} = (total number of σ bonds around each central atom + LP)

It is not possible to predict the hybridization state of the S atom in S_8 and the P atom in P_4 using a conventional formula, as shown in Figure 2.

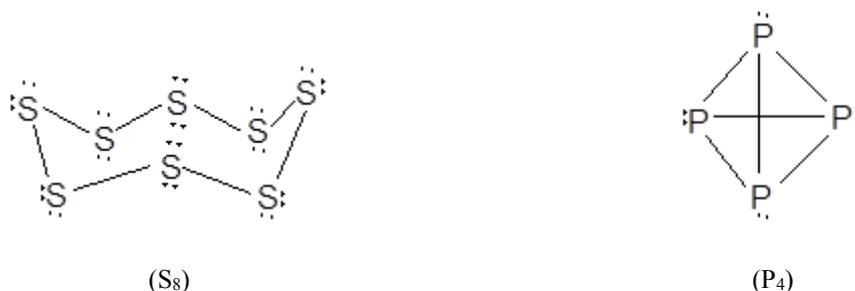


Figure 2. Zig-zag structure of S_8 and Tetrahedron structure of P_4

Example 2: The hybridization state of S in S_8

Conventional formula: $P = 1/2 (V+MA-C+A) = 1/2 (6+0-0) = 3.0$ (sp^2 - erroneous hybridization state of S in S_8)

Innovative formula: $(P_{Hyb}) = (T_{SLP}) - 1 = (2+2)-1 = 3$ (sp^3 hybridized S atom in S_8)

Where P_{Hyb} = power of the hybridization state of the central atom, and T_{SLP} = (total number of σ bonds around each central atom + LP)

Example 3: The hybridization state of P in P_4

Conventional formula: $P = 1/2 (V+MA-C+A) = 1/2 (5+0-0) = 2.5$ (unpredictable hybridization state of P in P_4)

Innovative formula: $(P_{Hyb}) = (T_{SLP}) - 1 = (3+1)-1 = 3$ (sp^3 hybridized P atom in P_4),

Where P_{Hyb} = power of the hybridization state of the central atom, T_{SLP} = (total number of σ bonds around each central atom + LP)

It is not possible to predict the hybridization state of a terminal carbon atom in alkynes using a conventional formula.

Example 4: The hybridization state of Ethyne, as presented in Figure 3.

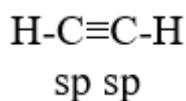


Figure 3. Linear structure of Ethyne (C_2H_2)

Conventional formula: $P = 1/2 (V+MA-C+A) = 1/2 (4+1-0) = 2.5$ (unpredictable hybridization state).

Innovative formula: $(P_{Hyb}) = (T_{SLP}) - 1 = 2-1 = 1$ (sp hybridized carbon atom in alkyne),

where P_{Hyb} = power of the hybridization state of the central atom, T_{SLP} = (total number of σ bonds around each central atom + LP)

Example 5: The hybridization state of pent-1-ene-4-yne, as presented in Figure 4.

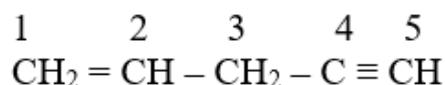


Figure 4. Structure of pent-1-ene-4-yne

Conventional formula: power of the hybridization state of the terminal carbon

$$C_5(P) = 1/2 (V+MA-C+A) = 1/2 (4+1-0) = 2.5 \text{ (unpredictable hybridization state } C_5).$$

Innovative formula: (P_{Hyb}) for $C_5 = (T_{SLP}) - 1 = 2 - 1 = 1$ (sp hybridized C_5),

Where P_{Hyb} = power of the hybridization state of the central atom, T_{SLP} = (total no of σ bonds around each central atom + LP)

It is not possible to predict the hybridization state of oxygen atoms in the cyclic ozone or hydrogen peroxide, the S atom in S_8 , or the P atom in P_4 using a conventional formula; however, using an innovative formula allows the hybridization state to be determined with absolute accuracy in all cases.

3.2. A comparative study between conventional and innovative formulae to predict the hybridization state of carbon atoms in different non-heterocyclic organic compounds

It is not possible to predict the hybridization state of carbon atoms in cyclopropene, cyclopentadiene, cycloheptatriene, cyclopropenyl anion, cyclopentadienyl anion, cycloheptatrienyl anion, cyclopropenyl cation, cyclopentadienyl cation, and cycloheptatrienyl cation, benzene, and toluene using a conventional formulae; however, using an innovative formula allows the hybridization state to be determined with absolute accuracy in all cases.

When a conventional formula was used the hybridization state of a vertex carbon atom in cycloalkenes, such as cyclopropene, cyclopentadiene, and cycloheptatriene, as shown in Figure 5, Figure 6, and Figure 7, it gave erroneous results.

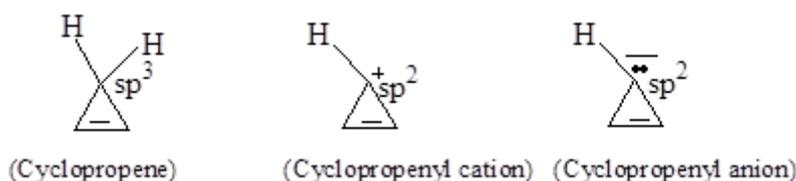


Figure 5. Structure of cyclopropene, cyclopropenyl cation, and cyclopropenyl anion

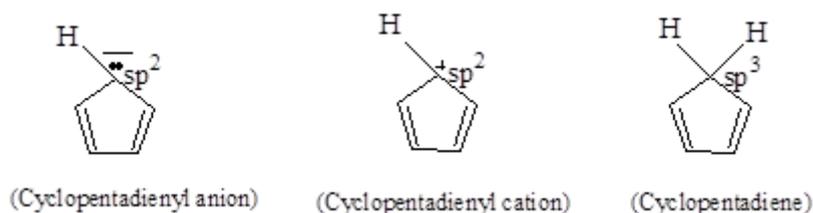


Figure 6. Structure of cyclopentadienyl anion, cyclopentadienyl cation, and cyclopentadiene

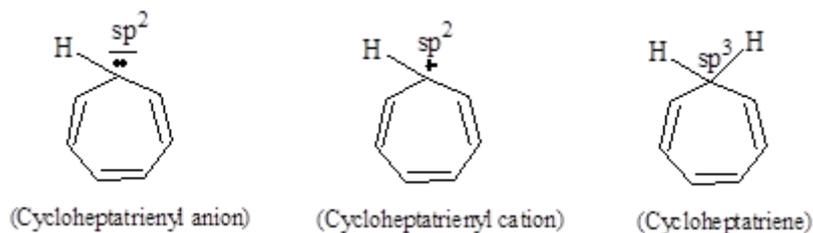


Figure 7. Structure of cycloheptatrienyl anion, cycloheptatrienyl cation, and cycloheptatriene

i) Conventional formula

The power of the hybridization state of the vertex carbon (P) = $1/2 (V+MA-C+A) = 1/2 (4+2-0) = 3$ (sp^2 - erroneous hybridization state).

ii) Innovative formula

Power of the hybridization state, (P_{Hyb}) = $(T_{SLNC}) - 1 = 4 - 1 = 3$ (sp^3 hybridization state of vertex carbon).

The hybridization state of carbon atoms, other than vertex carbon, in cycloalkenes, such as cyclopropene, cyclopentadiene and cycloheptatriene, Figure 5, Figure 6, and Figure 7, was unpredictable when using a conventional formula.

i) Conventional formula

The power of the hybridization state of the rest carbons (P) = $1/2 (V+MA-C+A)$ = $1/2 (4+1-0)$ = 2.5 (unpredictable hybridization state).

ii) Innovative formula

The power of the hybridization state was (P_{Hyb}) = (T_{SLNC}) - 1 = 3-1 = 2 (sp^2 hybridization state of rest carbons other than vertex carbon).

The hybridization state of vertex carbon atoms bearing a negative charge in cycloalkenyl anions, such as cyclopropenyl anion, cyclopentadienyl anion, and cycloheptatrienyl anion, Figure 5, Figure 6, and Figure 7, was erroneous when using a conventional formula.

i) Conventional formula

The power of the hybridization state of the vertex carbon (P) = $1/2 (V+MA-C+A)$ = $1/2 \{4+1-(0-1)\}$ = $1/2 \{6\}$ = 3 (sp^2 - erroneous hybridization state).

ii) Innovative formula

The power of the hybridization state of the vertex carbon is (P_{Hyb}) = (T_{SLNC}) - 1 = 3-1 = 2 (sp^2 hybridization state).

The hybridization state of a vertex carbon atom bearing a positive charge in cycloalkenyl cations, such as cyclopropenyl cation, cyclopentadienyl cation, and cycloheptatrienyl cation, Figure 5, Figure 6, and Figure 7, was erroneous when using a conventional formula.

i) Conventional formula

The power of the hybridization state in a vertex carbon bearing a positive charge, (P) = $1/2 (V+MA-C+A)$ = $1/2 \{4+1-(1+0)\}$ = $1/2 \{4\}$ = 2 (sp - erroneous hybridization state).

ii) Innovative formula

Power of the hybridization state of the vertex carbon bearing positive charge, (P_{Hyb}) = (T_{SLNC}) - 1 = 3-1 = 2 (sp^2 hybridization state).

The hybridization state of carbon atoms in benzene, toluene, and so on is unpredictable using a conventional formula but, when using an innovative formula, the hybridization state will be determined with absolute accuracy in all cases.

A carbon atom in benzene as illustrated in Figure 8

i) Conventional formula

The power of the hybridization state of carbon is (P) = $1/2 (V+MA-C+A)$ = $1/2 (4+1-0)$ = 2.5 (unpredictable hybridization state).

ii) Innovative formula

The power of the hybridization state of a carbon atom is (P_{Hyb}) = (T_{SLNC}) - 1 = 3-1 = 2 (sp^2 hybridization state).

Carbon atom from the methyl group in Toluene as illustrated in Figure 8

i) Conventional formula

The power of the hybridization state of a carbon atom from the methyl group in toluene is (P) = $1/2 (V+MA-C+A)$ = $1/2 (4+3-0)$ = 3.5 (unpredictable hybridization state).

ii) Innovative formula

The power of the hybridization state of a carbon atom from the methyl group in toluene is (P_{Hyb}) = (T_{SLNC}) - 1 = 4-1 = 3 (sp^3 hybridization state).

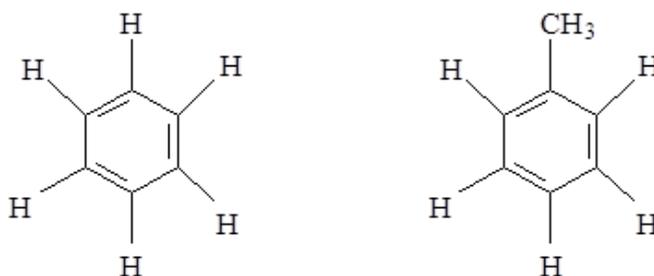


Figure 8. Structure of benzene and toluene

3.3. A comparative study between conventional and innovative formulae to predict the hybridization state of a heteroatom in different heterocyclic compounds

It is not possible to predict the hybridization state of heteroatom nitrogen in pyridine, quinoline, isoquinoline, pyrimidine, thiazole, benzothiazole, pyrazine, cyanidine, phenazine, 1,2,3,4-tetrazine, azocine, azetine, and aziridine, or an oxygen atom in oxetan using a conventional formula. However, when using an innovative formula, the hybridization state of a heteroatom in nitrogen will be determined with absolute accuracy in all cases.

i) Conventional formula

The power of the hybridization state of a nitrogen atom in pyridine is $P = 1/2 (V+MA-C+A) = 1/2 (5 + 0 - 0 + 0) = 2.5$ (unpredictable hybridization state) and the power of the hybridization state of a nitrogen atom in quinoline is $P = 1/2 (V+H-C+A) = 1/2 (5 + 0 - 0 + 0) = 2.5$ (unpredictable hybridization state) illustrated in Figure 9.

The power of the hybridization state of a nitrogen atom in aziridine is $P = 1/2 (V+MA-C+A) = 1/2 (5 + 1 - 0 + 0) = 3$ (sp^2 - erroneous hybridization state of N) and the power of the hybridization state of an oxygen atom in oxetan is $P = 1/2(V+MA-C+A) = 1/2 (6 + 0 - 0 + 0) = 3$ (sp^2 - erroneous hybridization state of oxygen atom) illustrated in Figure 10.

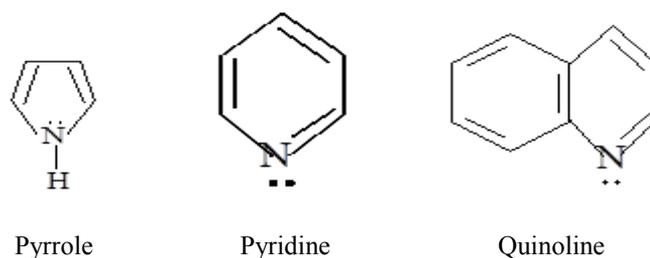


Figure 9. Structure of pyrrole, pyridine, and quinoline

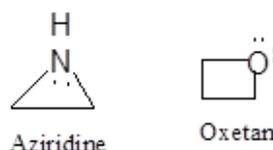


Figure 10. Structure of aziridine and oxetan

ii) Innovative formula

The power of the hybridization state of a heteroatom is $(P_{Hyb}) = (T_{SLLP}) - 1$.

The power of the hybridization state of a nitrogen atom in pyridine is $P_{Hyb} = (3 - 1) = 2$ (σ bonds = 2 & LLP = 1)

(sp^2 hybridization state of N atom) and the power of the hybridization state of a nitrogen atom in quinoline is $P_{Hyb} = (3 - 1) = 2$ (σ bonds = 2 & LLP = 1) (sp^2 hybridization state of N atom) illustrated in Figure 9.

The power of the hybridization state of a nitrogen atom in aziridine is $P_{Hyb} = (4 - 1) = 3$ (σ bonds = 3 & LLP = 1)

(sp^3 hybridization state of N atom) and the power of the hybridization state of an oxygen atom in oxetan is $P_{Hyb} = (4 - 1) = 3$ (σ bonds = 2 & LLP = 2) (sp^3 hybridization state of O atom) illustrated in Figure 10.

4. CONCLUSION

In this article, the limitations of conventional formulae have been discussed in the light of innovative formulae to predict the hybridization state of simple molecules or ions and organic compounds, including heterocyclic compounds. Educators can use this comparative study in their classroom lectures to make chemistry intriguing and trustworthy.

REFERENCES

Predicting the hybridization state: a comparative study between conventional and innovative ... (Arijit Das)

- [1] L. Pauling, "The Nature Chemical Bond. Application of Results Obtained from the Quantum Mechanics and from a Theory of Paramagnetic Susceptibility to the Structure of Molecules," *Journal of American Chemical Society*, vol. 53, no. 4, pp. 1367-1400, 1931.
- [2] L. Pauling, *et al.*, "Chemistry," *Freeman International Ed.*, pp. 148, 163-167, Toppan, Japan, 1975.
- [3] L. Pauling, *The nature of the chemical bond*, 3rd ed., Cornell University Press, Ithaca., N. Y., pp. 85,189, 1960.
- [4] J. S. Wright, "Theoretical Evidence for a Stable form of Cyclic Ozone, and its Chemical Consequences," *Can.J.Chem.*, vol. 51, pp. 139-146, 1973.
- [5] J.E.Huheey, *et al.*, *Inorganic Chemistry*, 4th ed., PEARSON, India, pp. 172-185, 2012.
- [6] I.L. Finar, *Organic Chemistry*, vol-2, 5th ed., Pearson, pp. 606-637, 2002.
- [7] R.T. Morrison, *et al.*, *Organic Chemistry*, 6th ed., pp. 1059-1061, 1992.
- [8] T.W.Graham Solomons, *et al.*, *Organic Chemistry*, 9th ed., Wiley: India, pp.655-658, 2012.
- [9] J.G. Smith, *Organic Chemistry*, 2nd ed., pp. 616-619, 2008.
- [10] Jerry March, *Advanced Organic Chemistry: Reaction, Mechanisms and Structure*, 4th ed. A Willy-Interscience Publication, JOHN WILEY & SONS, New York, p.45, 2005.
- [11] A.Bahl, *et al.*, *A Text Book of Organic Chemistry*, 22nd ed., S.Chand & Company Pvt.Ltd., New Delhi, India, pp. 900-920, 2016.
- [12] B.M. Mahan., *et al.*, *International Student Edition University Chemistry*, 4th ed., pp. 599-603, 1998.
- [13] B. Douglas., *et al.*, *Concepts and Models of Inorg. Chem.*, 3rd ed., Wiley India, pp. 157, 38, 2007.
- [14] F.A. Cotton., *et al.*, *Basic Inorg.Chem.*, 3rd ed., Wiley India, pp. 107, 111, 523, 2007.
- [15] R.L. Dutta, *Inorg. Chem.*, 6th ed., pp. 146-147, 2009.
- [16] R.L. Madan, *A Text Book of Chemistry*, 1st ed., p88, 2011.
- [17] S.M.Mukherji, *et al.*, *Org. Chem.*, 2nd ed., New Age Int. Pub., vol. 1, pp. 1-11, 2013.
- [18] M.K.Jain, *et al.*, *Modern Org. Chem.*, pp. 37-41, 2017
- [19] S.K.Agarwal, *et al.*, *Advanced Inorg. Chem.*, 17th ed., pp. 64-78, 2019.
- [20] J.D. Lee, *Concise Inorg.Chem.* Wiley: India and Oxford, 5th ed. pp. 944, 109-112, 2008
- [21] A. Das, "A Review of Time Economic Innovative Mnemonics In Chemical Education," *International Journal of Physics & Chemistry Education (Eurasian Journal of Physics and Chemistry Education - EJPCE)*, vol. 10, no. 1, pp. 27-40, 2018.
- [22] A. Das, "Innovative Mnemonics In Chemical Education: Review Article," *African Journal of Chemical Education(AJCE)*, vol. 8, no. 2, pp. 144-189, 2018.
- [23] A. Das, "Innovative Mnemonics Make Chemical Education Time Economic – A Pedagogical Review Article", Special Issue "Teaching Science in the 21st Century," *World Journal of Chemical Education (WJCE)*, vol. 6, no. 4, pp. 154-174, 2018.
- [24] A. Das, "Lone Pair Electron Discriminate Hybridization with Aromatic and Anti Aromatic behavior of Heterocyclic Compounds-Innovative Mnemonics," *World Journal of Chemical Education (WJCE)*, vol. 6, no. 2, pp. 95-101, 2018.
- [25] A. Das, "Review of Innovative Mnemonics for Inorganic and Organic Chemical Education," *Chemistry Journal, American Institute of Science (AIS)*, vol. 4, no. 2, pp. 11-31, 2018.
- [26] A. Das, "Innovative Mnemonics in Chemical Education - A Review Article," *American Journal of Chemistry and Applications. Open Science*, vol. 5, no. 1, pp. 19-32, 2018.
- [27] A. Das, "Innovative And Time Economic Pedagogical Views In Chemical Education - A Review Article," *World Journal of Chemical Education*, vol. 2, no. 3, pp. 29-38, 2014.

BIOGRAPHY OF AUTHOR



Dr Arijit Das is the Assistant Professor of the Department of Chemistry at Bir Bikram Memorial College (BBMC), India, having received his Ph.D. from Tripura Central University, India, in 2008. He is a member of the Chemical Education Division of the American Chemical Society, and a Life-Time Fellow of the Directorate of Chemical Science, as recognized by the International Agency for Standards and Ratings, which also mentioned him among the world's "500 Most Influential Experts in Chemical Science" in 2018. Dr. Das was an author and presently is a member of 'Chemistry Editorial Advisory Board', Cambridge Scholars Publishing, England, UK. His biography included from the 'Wikipedia' in the 'Wiki bios', UK On dated 19th April 2019, (Link: https://en.everybodywiki.com/Arijit_Das).